

Geometrical universality in vibrational dynamics

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(February 1, 2008)

A good generalization of the Euclidean dimension to disordered systems and non crystalline structures is commonly required to be related to large scale geometry and it is expected to be independent of local geometrical modifications. The spectral dimension, defined according to the low frequency density of vibrational states, appears to be the best candidate as far as dynamical and thermodynamical properties are concerned. In this letter we give the rigorous analytical proof of its independence of finite scale geometry. We show that the spectral dimension is invariant under local rescaling of couplings and under addition of finite range couplings, or infinite range couplings decaying faster than a characteristic power law. We also prove that it is left unchanged by coarse graining transformations, which are the generalization to graphs and networks of the usual decimation on regular structures. A quite important consequence of all these properties is the possibility of dealing with simplified geometrical models with nearest-neighbors interactions to study the critical behavior of systems with geometrical disorder.

On translationally invariant structures such as crystals, many physical phenomena fundamentally depend on the Euclidean dimension d , regardless of the particular form of elementary cells. This parameter appears to resume all relevant informations about large scale geometry and therefore it affects the dynamics at low frequencies as well as the thermodynamics at low temperatures and near critical points. In fact this relation is one of the deepest aspects of the physics of systems with many degrees of freedom. Even if it has not been proved yet in general, it is commonly accepted and it is experimentally found that this dimensional dependence is not modified when translational invariance is lost as a consequence of inhomogeneities or disorder at finite scales. This invariance under couplings disordering and local changes in geometry, which we call *geometrical universality*, is perhaps the most important feature of dimension in statistical physics. Therefore it is quite reasonable to require that it is preserved in any meaningful generalization of the Euclidean dimension.

The spectral dimension \bar{d} , firstly introduced by Alexander and Orbach [1] to characterize the low frequency vibrational spectrum of fractals, is considered for many reasons the right generalization of d to non-crystalline structures such as polymers, glasses, fractals, amorphous materials and so on. In fact \bar{d} exactly replaces d in most laws where dimensional dependence explicitly appears: the spectrum of harmonic oscillations, the average autocorrelation function of random walks, the critical exponents of the spherical model [2], the low temperature specific heat, the generalized Mermin-Wagner theorem [3], the infrared singularities of the Gaussian model and many others. In addition \bar{d} can be easily measured by well known experimental techniques such as e.g. neutron scattering. These remarkable properties suggest extending to non-crystalline structures the same picture holding for crystals. In other words, we expect that, even on non translationally invariant networks, the fundamental physical properties depend only on large scale geometry and that all this dependence is encoded in \bar{d} . This would mean that all we need to deal with geometrical disorder is a non-integer parameter generalizing the usual dimension and it also would mean that geometrical disorder does not imply complex behavior. Clearly, such an appealing picture strongly depends on universal properties of \bar{d} which are not obvious neither proved yet. The rigorous proof of these properties is the subject of this letter.

After introducing the basic concept and notations concerning \bar{d} , we will prove its geometrical universality following three major steps, modifying the networks by acting on the strength of links, on the number of links and on the number of points. First, \bar{d} is proved to be invariant under a bounded local rescaling of couplings, which therefore does not alter the underlying geometry. Then we will prove its invariance under the addition of finite range and infinite range couplings up to a characteristic power law decay, changing in this way the geometrical structure under consideration by modifying an infinite number of links. Finally we will consider a general coarse graining procedure, which changes the number of degrees of freedom of the network while leaving \bar{d} invariant. These general transformations allow to group very different networks under the same geometrical universality class, characterized by a given value of \bar{d} . Their significance and applications will be discussed in details in the conclusions.

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The spectral dimension of an infinite connected graph G can be defined by studying the low frequency behavior of its vibrational spectrum. A graph is a set of points with a topology described by its adjacency matrix A_{ij} , whose elements are equal to 1 if the points i and j are nearest neighbors and equal to 0 in all other cases.

This mathematical structure can be used as a geometrical model for an oscillating network with masses m at each point, connected along the links by springs with elastic constant k . Introducing the positive definite Laplacian operator $L_{ij} \equiv z_i \delta_{ij} - A_{ij}$, $z_i = \sum_j A_{ij}$ being the coordination number of site i , the eigenvalue equations for the vibrational normal modes read

$$k \sum_j L_{ij} x_j = \omega^2 m x_i \quad (1)$$

where ω is the frequency and x_i the displacement from equilibrium position at site i . The spectral dimension \bar{d} is then defined by the asymptotic behavior of the density of modes with frequency ω , $\rho_\omega(\omega) \sim \omega^{\bar{d}-1}$ for $\omega \rightarrow 0$. By (1), the spectral dimension is related to the density $\rho_l(l)$ of eigenstates of the Laplacian with eigenvalue l , whose behavior is given by $\rho_l(l) \sim l^{\bar{d}/2-1}$ for $l \rightarrow 0$. This relation gives the basis to describe large scale properties of statistical models in terms of \bar{d} . In particular, we shall consider the Gaussian model, which provides the most effective tools to deal with universal properties of \bar{d} .

The Gaussian model on G is defined by the Hamiltonian:

$$H = \frac{1}{2} \sum_{ij} \phi_i (L_{ij} + m^2 \delta_{ij}) \phi_j \quad (2)$$

and its specific free energy f is given by

$$f = - \lim_{N \rightarrow \infty} \frac{1}{N} F = - \lim_{N \rightarrow \infty} \frac{1}{N} \log Z \quad (3)$$

where Z is the partition function calculated according to the Boltzmann weight $\exp(-H)$. Its correlation functions are given by

$$\langle \phi_i \phi_j \rangle = (L + m^2)^{-1}_{ij} \quad (4)$$

and from (4) the matrix $\Phi_{ij} \equiv \langle \phi_i \phi_j \rangle$ is positive definite. The spectral dimension is related to the singular part of f for $m^2 \rightarrow 0$ by:

$$Sing(f) \sim m^{\bar{d}}. \quad (5)$$

Using this definition of \bar{d} and the above mentioned properties, a “weak” universality of \bar{d} has been proved, namely its independence of a local bounded rescaling of masses [4], showing that (5) is left invariant replacing m^2 by $m_i^2 = \alpha_i m^2$ in (2), with $K^{-1} < \alpha_i < K$ for some $K > 1$.

Now our first step is the extension of such invariance to a local bounded rescaling of couplings. Such “stronger” universality will provide the mathematical basis for all further points. First of all, we notice that a global rescaling of all couplings by a given constant c does not affect \bar{d} , since it is equivalent to a global mass and correlation functions rescaling. Then we prove the invariance of (5) under the rescaling $A_{ij} \rightarrow J_{ij} = c_{ij} A_{ij}$, with $K^{-1} < c_{ij} < K$, corresponding to the generalized Laplacian $L'_{ij} \equiv z'_i \delta_{ij} - J_{ij}$, $z'_i = \sum_j J_{ij}$. The strategy consists in taking successive derivatives of (5) with respect to m^2 up to a divergence for $m^2 \rightarrow 0$, in proving the monotonicity of such derivatives with respect to a generic local increasing of the couplings J_{ij} and then exploiting their boundedness between the two limit cases of global rescaling $J_{ij} = K^{-1}$ and $J_{ij} = K$. The key point is the monotonicity relation

$$- \sum_{kl} a_{kl} \frac{\partial}{\partial J_{kl}} \left(- \frac{\partial}{\partial m^2} \right)^n f \geq 0 \quad (6)$$

holding for $a_{kl} \geq 0$ and every $n \geq 1$. This can be proved by noticing that

$$- \frac{\partial}{\partial J_{kl}} \left(- \frac{\partial}{\partial m^2} \right)^n F = (\Phi^n)_{kk} + (\Phi^n)_{ll} - 2(\Phi^n)_{kl} \quad (7)$$

and that the right hand side of (7) is the value of a positive definite quadratic form computed on two coinciding vectors v , namely $\sum_{ij} v_i (\Phi^n)_{ij} v_j$, with $v_i = \delta_{ik} - \delta_{il}$.

This first theorem (which we will call *strong universality theorem* or SUT) proves that \bar{d} depends only on topology and is not affected by possible disorder in interactions strengths and, together with the previous result [4] concerning rescaling of masses, shows that the low frequency vibrational spectrum is only related to geometry. In the following, we will see that indeed only *large scale* geometry comes into play. The second and third steps deal with transformations affecting the topology itself, implying a change in the number of links and points. It is clear that the changes we are considering must involve sets of links or points having non vanishing density in the whole graph in the thermodynamic limit. Indeed, changing a finite number of entry in the Laplacian, or an infinite one with zero density, corresponds to a compact perturbation and therefore does not modify its continuous spectrum [5].

The simplest transformation on links is the addition of bounded next to nearest neighbor interactions (NNI). Their exact values are clearly irrelevant due to SUT. A possible system G' with such additional interaction is described by the generalized Laplacian $L'_{ij} = cL_{ij} - (L^2)_{ij}$, with $c > 2z_{max}$, which is second degree polynomial in L_{ij} lacking of the constant term. Its eigenvalues l' are related to the eigenvalues l of L by $l' = cl - l^2$ and they become asymptotically proportional for $l \rightarrow 0$. This implies the asymptotic coincidence of the respective spectral density and, therefore, the invariance of \bar{d} . Now, due to SUT, a generic graph obtained from G by adding some (not necessarily all!) NNI has the same spectral dimension too. This proof is easily extended to the addition of interactions up to an arbitrary finite distance q . Indeed, iterating n times the same NNI transformation on G' , one obtains a system with interactions to all distances up to 2^{n+1} . Choosing a suitable n , the invariance of \bar{d} follows from SUT. Now, consider the inverse transformation, consisting in acting on G cutting bonds which are limited range couplings with respect to the topology of the resulting graph G' . We shall call it *bond cutting transformation* (BCT). From its definition, it follows that BCT preserve \bar{d} . This property will be very useful in the following.

An analogous strategy can be used to show the invariance of \bar{d} under the introduction of a long range interaction, with power law or exponential decreasing in the graph chemical distance r . The fundamental observation is that, when the asymptotic behavior of the eigenvalues l' of the generalized long range Laplacian L' is given by $l' = cl + l^\alpha$, with $\alpha > 1$, the new interaction does not modify \bar{d} , since the above exploited proportionality still holds.

Now, if the long range interaction decreases as $r^{-\gamma}$, where $\gamma > d_c$ (d_c being connectivity dimension of G) as required by local energy finiteness, it can be shown, expanding L' on the basis of the eigenvectors of L , that $\alpha = d(\gamma - d_c)/2d_c$. Therefore \bar{d} is left unchanged by power law interactions with $\gamma > d_c + 2\frac{d_c}{d}$ and, from SUT, by any exponential decaying interaction. Notice that on Euclidean lattices, where $d_c = \bar{d} = d$, this reproduces the well known result $\gamma > d + 2$. The addition of a power law interaction with a slower decay always alter \bar{d} . From the previous considerations, \bar{d} increases according to $\bar{d}' = 2d_c/(\gamma - d_c)$.

The class of transformations considered up to now does not modify the number of points of G .

The last kind of graph modifications we will analyze involves a non trivial change in the number of degrees of freedom. Actually they include one of the most important class of transformations used in statistical mechanics, namely decimations, which are the basic tool of renormalization group on lattices and fractals.

We call these transformations *topological rescalings*, since they generate local changes in the number of points. The most general topological rescaling can be realized through two independent steps. The first one is the *partition* and consists in dividing the graph G in an infinite family of connected subgraphs G_α , with uniformly bounded number of points. The second one is the *substitution* and consists in generating a new graph G' by replacing some or all G_α by a different (connected) graph S_α , whose number of points ranges from 1 to a fixed N_{max} , and by adding links connecting different S_α in such a way that two generic S_α and S_β are connected by some links if and only if G_α and G_β were. The simplest topological rescaling occurs when every S_α is composed by just one point. In this case the resulting graph G_m is called the *minimal structure* of the partition $\{G_\alpha\}$. The invariance of \bar{d} under topological rescaling can be reduced to proving that G and the minimal structures of its partitions have the same \bar{d} . Indeed, from this property it easily follows that two graphs having the same minimal structure also have the same \bar{d} and it can be proven that G and G' have the same minimal structure. We will now show that \bar{d} is left unchanged reducing G to its minimal structure.

For every subgraph G_α let us define the boundary of G_α , ∂G_α , as the set of points of G_α which are connected to at least one point of G_β , $\beta \neq \alpha$. We will call M_α the number of points of ∂G_α . Let us consider a new graph G' obtained by replacing each subgraph G_α with the complete graph of its boundary points, K_{M_α} (the complete graph K_n is the n -points graph with each point connected to all the other ones). It can be shown [6] that, considering the Gaussian model (2) on G and the Gaussian model on G' with suitable bounded masses m'_i , defined on the points of the ∂G_α 's and bounded couplings J'_{ij} , between the points of K_{M_α} , one has for the free energies defined on the two graphs G and G' :

$$f_G = f_{G'} \quad (8)$$

The geometry of the new graph G' can be further simplified applying the previous transformations. First, since we are interested in the singular part of f , the exact values of the bounded masses and couplings between the points of

K_{M_α} are irrelevant due to SUT.

Now consider a single K_{M_α} together with the K_{M_β} which are connected to it. Then for every K_{M_β} select one point $i_\alpha(\beta)$ among the $M_\alpha(\beta)$ points connected to K_{M_β} and cut the links between all the other $M_\alpha(\beta) - 1$ points and K_{M_β} using BCT.

Applying again the bonds cutting transformation, one can reduce the $i_\alpha(\beta)$ points to a linear chain, observing that all the other links can be considered as couplings up to k -th neighbors with respect to nearest-neighbors interactions between points of the linear chain.

The linear chains can now be shrunked to one point p_α by first applying the previously mentioned Gaussian model reduction [6], leading to a new relation for the free energies as in (8), and then cutting the spurious links between external points added with this operation using BCT.

Therefore, one is left with a single point p_α for each G_α connected to the p_β corresponding to those subgraphs G_β whose points were connected to G_α in G . This graph G_m precisely corresponds to the minimal structure of the initial partition of G and it has the same \bar{d} as G .

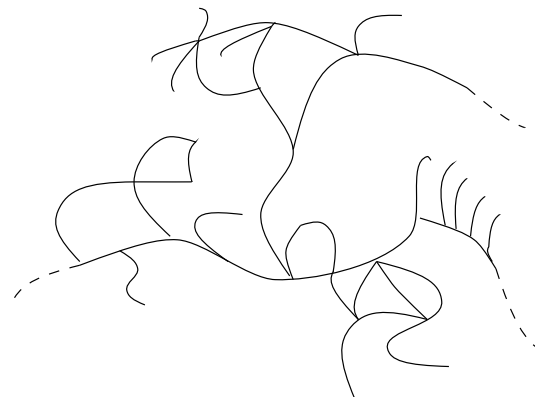
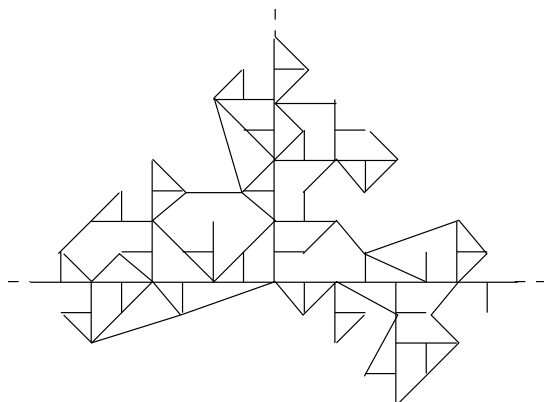
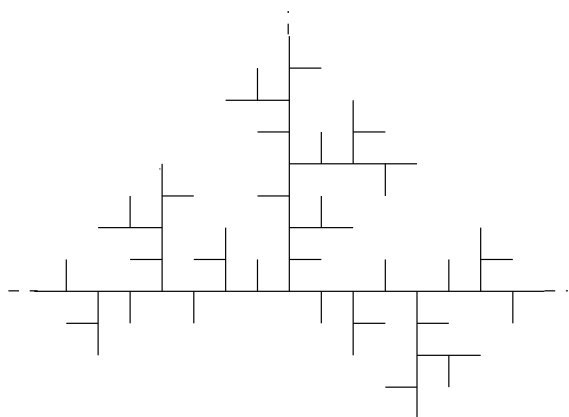
The three very general classes of geometrical transformations we have been considering can be applied in all possible sequences to a graph, leading to an overall transformation on coupling strength, number of links and degrees of freedom which does not change its spectral dimension \bar{d} . We will call such a transformation an *isospectrality*. Interestingly enough, isospectralities include a well known class of transformations on graphs studied in graph theory, namely the rough-isometries [7].

Indeed, isospectralities include most part of currently used transformations. As an example, the usual decimation procedure on fractals is a topological rescaling. In particular, for all exactly decimable fractals (such as e.g. Sierpinski gaskets and T-fractals [8]), the minimal structure of the graph coincides with the graph itself. Again, an isospectrality relates the usual two dimensional square lattice, the hexagonal lattice and the triangular lattice, which therefore all have dimension 2. In other words, isospectralities are the theoretical formalization of the intuitive idea of invariance with respect to bounded scale perturbations and disorder and the *isospectrality classes*, defined as the classes of graphs related by such transformations, are the practical realization of the apparently abstract concept of non integer dimension. Now, since most dynamical and thermodynamical properties of generic discrete structures depend only on \bar{d} , isospectralities provide a very powerful tool to reduce a very complicated geometrical structure to the simplest one having the same \bar{d} . The latter turns out to be much simpler to study and still presents the same universal properties. Moreover, not only an isospectrality can be used to reduce and simplify structures and problems. It can also be applied, with the opposite aim, to build complicated structures with controlled dynamical and thermodynamical properties, starting from simple deterministic geometrical models. This is the point of view of *spectral dimension engineering*, providing a very interesting field of possibilities to polymer physicists and material scientists dealing with non-crystalline materials.

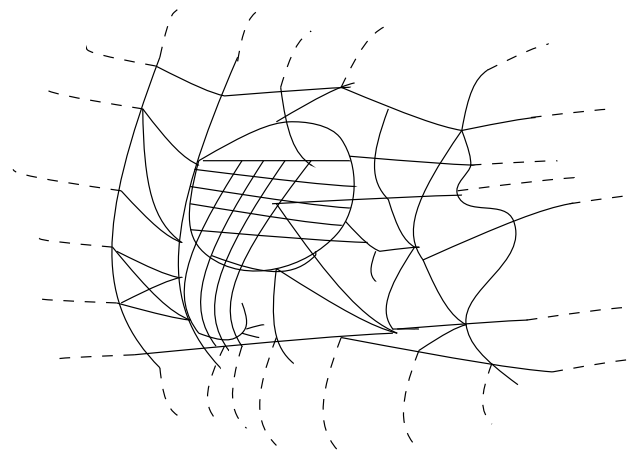
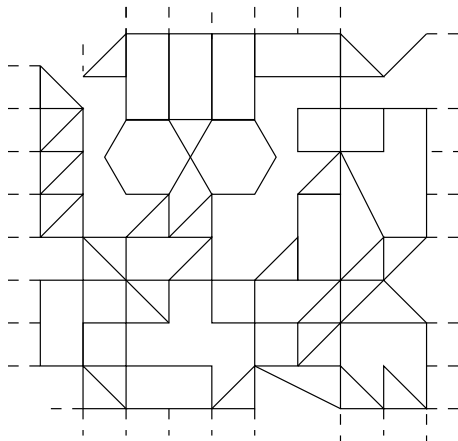
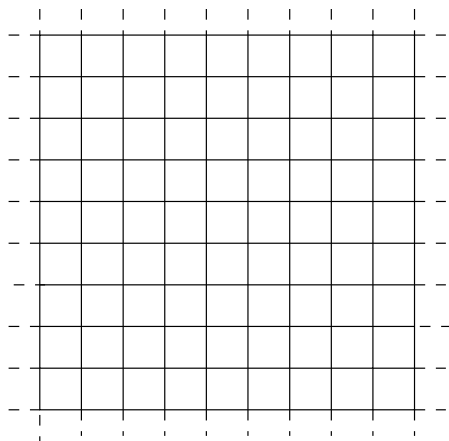
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Figure caption

Fig.1: Example of isospectral structures obtained applying isospectral transformations (without long range couplings) to the T-fractal (a) and to the square lattice (b).



a)



b)